

Guanidine, N,N''-(iminodi-8,1-octanediyl)bis-
13516-27-3 | DTXSID7042015

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 8650 L/kg

Global applicability domain: Outside

Local applicability domain index: 2.22e-01

Confidence level: 6.31e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Di(2-ethylhexyl) adipate</div> <div>Measured: 15500</div> <div>Predicted: 14400</div>	<div>Image not found</div> <div>Dioctyl phthalate</div> <div>Measured: 24000</div> <div>Predicted: 17100</div>	<div>Image not found</div> <div>Bis(2-ethylhexyl) terephthalate</div> <div>Measured: 14500</div> <div>Predicted: 12500</div>
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